

# Numerical and Monte Carlo Bethe ansatz method: 1D Heisenberg model

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In this paper we present two new numerical methods for studying thermodynamic quantities of integrable models. As an example of the effectiveness of these two approaches, results from numerical solutions of all sets of Bethe ansatz equations, for small Heisenberg chains, and Monte Carlo simulations in quasi-momentum space, for a relatively larger chains, are presented. Our results agree with those obtained by thermodynamics Bethe ansatz (TBA) and Quantum Transfer Matrix (QTM).

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## I. INTRODUCTION

The study of exactly solvable models is a very important field in condensed matter physics, which began with Bethe's solution of the isotropic Heisenberg chain [1]. In general, the Bethe ansatz (BA) solution of a model has several drawbacks: it has a complex mathematical structure; the excitations are not immediately available; and most important, it does not give explicit results even for the thermodynamic quantities of the system. It was only when Yang and Yang [2] presented a strategy to study the thermodynamics of BA solvable systems that the temperature dependence of quantities such as the specific heat and the magnetic susceptibility become available. The method is now designated as thermodynamic Bethe ansatz and has known many developments in the last thirty years [3]. Additionally, correlation functions, such as the conductivity, can not be obtained from the BA equations alone, and combination of BA results with other methods is required for their calculation [4].

The BA ansatz method has been applied to Bose, Fermi [5, 6, 8], and spin systems [1, 7]. It is a general feature of the BA solution, first proved by Yang and Yang[2] for the Bose case, that a given eigenstate of the model is characterized by a unique set of quantum numbers  $\{I_j\}$ . Further, it also can be shown that all configurations of these quantum numbers  $I_j$  exhaust the Hilbert space of a given model. Since the energy eigenvalues are functions of the above quantum numbers, instead of using TBA and quantum Monte Carlo approaches, we can study BA solvable models in quantum number space by classical Monte Carlo. Furthermore, for a small system (but for larger systems than those available to exact diagonaliza-

tion methods), it is possible to solve the BA equations for all eigenvalues. Therefore, the expectation value of an Hermitian operator in thermal equilibrium can be computed.

In this paper, we shall introduce two numerical approaches for computing thermodynamic quantities of Bethe ansatz solvable models. The methods are illustrated with the 1D isotropic Heisenberg model, since this model is well studied in the literature. Furthermore, the study of the Heisenberg model is it self relevant, since this system predicts many properties of quasi-one-dimensional materials [10, 11, 12]. This model has been investigated by many kinds of methods. For example, the low temperature behaviors are quite well understood by a combination of Bethe ansatz [13] and conformal field theory [14, 15]. A strong logarithm singularity in the susceptibility at low temperature was first found by the Bethe ansatz calculation of quantum transfer matrix [16] and then verified experimentally [10, 11]. The thermodynamics of the model has been studied by TBA [3, 17, 18, 19, 20, 21, 22] as well as by QTM [23, 24, 25, 26].

The paper is organized as follows. In Sec. II, we first briefly review the BA solution of the isotropic Heisenberg model. In Sec. III and Sec. IV, we introduce the basic idea of numerical Bethe ansatz (MBA) and Monte Carlo Bethe ansatz (MCBA). In Sec.V we check the effectiveness of these two methods computing the specific heat and the magnetic susceptibility in the absence of an external magnetic field and compare our results with those obtained from the TBA. We than use our methods to study the two quantities above in the presence of an external magnetic field. A brief summary is given in Sec. VI.

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## II. ISOTROPIC HEISENBERG MODEL

Now let us first review the Bethe ansatz solution of the 1D Heisenberg chain, which can be found in the book of Takahashi [3]. The Hamiltonian of the isotropic Heisenberg model is

$$\mathcal{H} = -J \sum_{l=1}^N (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + S_l^z S_{l+1}^z), \quad (1)$$

where  $N$  is the number of sites,  $S_l^x, S_l^y, S_l^z$  are spin  $1/2$  operators at site  $l$  and  $J = -1, 1$  represent anti-

ferromagnetic and ferromagnetic cases, respectively. The solution with periodic boundary condition  $\tilde{S}_{N+1} = \tilde{S}_1$  using the string hypothesis takes the form

$$N\theta(x_\gamma^n/n) = 2\pi I_\gamma^{(n)} + \sum_{m, \beta \neq n, \gamma} \Theta_{nm}(x_\gamma^n - x_\beta^m). \quad (2)$$

Here  $\theta(x) = 2 \tan^{-1}(x)$ , and

$$\begin{aligned} \Theta_{nm}(x) &= \theta\left(\frac{x}{|n-m|}\right) + 2\theta\left(\frac{x}{|n-m|+2}\right) + \cdots + 2\theta\left(\frac{x}{n+m-2}\right) + \theta\left(\frac{x}{n+m}\right) \quad \text{For : } n \neq m \\ &= 2\theta\left(\frac{x}{2}\right) + 2\theta\left(\frac{x}{4}\right) + \cdots + 2\theta\left(\frac{x}{2n-2}\right) + \theta\left(\frac{x}{2n}\right) \quad \text{For : } n = m \end{aligned} \quad (3)$$

and  $x_\gamma^n$  is the real part of the  $n$ -string which is designated by

$$x_\gamma^{n,j} = x_\gamma^n + i(n+1-2j), \quad j = 1, \dots, n$$

$I_\gamma^n$  is the quantum number of  $\gamma$ th  $n$ -string (note that  $n$  and  $\gamma$  are indices). We denote the number of the  $n$ -string by  $\alpha_n$ , thus  $\gamma = 1, \dots, \alpha_n$  and the string configuration  $\{\alpha\}$  satisfy

$$\alpha_1 + 2\alpha_2 + \cdots + (M-1)\alpha_{M-1} + M\alpha_M = M, \quad (4)$$

where  $M$  is the number of down spins. The quantum number of  $n$ -string  $I_\gamma^n$  is an integer (half-odd integer) if  $N - \alpha_n$  is odd (even) and satisfy

$$|I_\alpha^n| \leq (N-1 - \sum_{m=1}^M t_{nm}\alpha_m)/2, \quad (5)$$

where  $t_{nm} \equiv 2 \min(n, m) - \delta_{nm}$ . For a given set of  $\{I_\gamma^n\}$ , Eq. (2) can be solved numerically and the energy is given by

$$E\{I_\gamma^n\} = -NJ/4 + \sum_{n, \gamma} \frac{2Jn}{(x_\gamma^n)^2 + n^2}, \quad (6)$$

which represents the energy of the lowest weight state in  $SU(2)$  irreducible space designated by  $S = N/2 - M, S_z = S, S-1, \dots, -S$ . In the presence of an external field  $h$  a Zeeman term is added to Eq. (6). Hence the total energy of a given quantum number configuration is given by

$$E = E\{I_\gamma^{(n)}\} - h\mathcal{M}, \quad (7)$$

where  $\mathcal{M} = 2S_z$  is the magnetization of the state

## III. NUMERICAL BETHE ANSATZ

In statistical mechanics, the expectation value of an Hermitian operator  $Q$  in thermal equilibrium is given by

$$\langle Q \rangle = \frac{1}{Z} \sum_{\mu} Q_{\mu} e^{-\beta E_{\mu}}. \quad (8)$$

where  $Z$  is known as partition function, defined as

$$Z = \sum_{\mu} e^{-\beta E_{\mu}}, \quad (9)$$

$\beta$  is inverse temperature, and  $\sum_{\mu}$  represents sum over all possible eigenstates of the Hamiltonian. It turns out that the variation of  $Z$  with respect to temperature or any other external parameters affecting the system can virtually tell us everything we might want to know about the macroscopic behavior of the system. For example, the internal energy is given by

$$U = \frac{1}{Z} \sum_{\mu} E_{\mu} e^{-\beta E_{\mu}} \quad (10)$$

From Eq. (9), it is easy to see that the internal energy can also be written in terms of a derivative of the partition function:

$$U = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\partial \ln Z}{\partial \beta}. \quad (11)$$

The specific heat is given by the derivative of the internal energy:

$$C_v = \frac{\partial U}{\partial T} = -k_B \beta^2 \frac{\partial U}{\partial \beta} = -k_B \beta^2 \frac{\partial^2 \ln Z}{\partial \beta^2}. \quad (12)$$

where  $k_B$  is the Boltzmann constant which is set to unit hereafter.

Our aim is to combine the idea of statistical mechanics mentioned above with the numerical solution of the BA equations. The main idea of the numerical Bethe ansatz method we introduce here is, first, to compute all eigenvalues of a BA solvable model from its corresponding BA equations. Then to compute the expectation value of the Hermitian operators, representing the physical observables we are interested in, by averaging those operators over all states of the system, weighting each state with its own Boltzmann weight.

It has been shown [3] that the Hilbert space of the isotropic Heisenberg model is complete under the string classification. Here we want to show how to travel through all  $C_{N/2}^N$  states in quantum number space and illustrate it by considering a system of 6 sites.

For the case of  $M$  down spins, the first task is how to obtain all string configurations fulfilling the restriction (4). We adopt a time-like number “ $\alpha_M : \alpha_{M-1} : \dots : \alpha_2 : \alpha_1$ ”, where the magnitude  $\alpha_n$  measures from 0 to  $[M/n]$  (here  $[x]$  returns the truncated integer value of  $x$ ), just like hour and minute in “HH:MM” measure from 0 to 23 and 0 to 59 respectively. If we increase the number “ $\alpha_M : \dots : \alpha_1$ ” by adding 1 to the first digit  $\alpha_1$  step by step, we can travel through all possible values. Among all these numerical values, only those whose digits satisfy the condition (4) are what we need. Then all string configurations can be found by this procedure. Of course, these operations are realized in a computer. In order to make the method clear, let us consider a problem of 6 sites.

**M=0:** It is easy to have the state with all spins up, i. e.  $M = 0$ , which has energy  $E = -JN/4$ .

**M=1:** In this case, we only have one string configuration  $\alpha_1 = 1$  and one quantum number  $-2 \leq I_1 \leq 2$ , thus there are 5 states. Each of them is represented by one quantum number in the interval  $[-2, 2]$ . We can get all possible quantum number configurations from the following figure,

$$- - \circ - - \circ - - \bullet - - \circ - - \circ - -$$

where the dot is the occupied quantum number, and the open circles represent other possible quantum numbers. Then the BA equation is just

$$6 \tan^{-1} x_1^1 = \pi I_1, \quad (13)$$

which has a simple solution  $x_1 = \tan(\pi I_1/6)$ .

**M=2:** Here the string configuration is characterized by  $\{\alpha_1, \alpha_2\}$ . We construct a number “ $\alpha_2 : \alpha_1$ ”, in which the maximum value of  $\alpha_1$  is 2 ( $[2/1] = 2$ ), and  $\alpha_2$  1 ( $[2/2] = 1$ ). Increasing  $\alpha_1$  step by step we generate all possible configurations of the “ $\alpha_2 : \alpha_1$ ” number, ranging from 0:0 to 1:2. Among all the generated configurations, we are only interested in those satisfying the condition  $\alpha_1 + 2\alpha_2 = 2$ . The first case is  $\alpha_1 = 2, \alpha_2 = 0$ , in which the quantum number satisfy  $-1.5 \leq I_1^1, I_2^1 \leq 1.5$ ,

TABLE I: All quantum number configurations for  $M = 2$ .

$\alpha_1 = 2, \alpha_2 = 0$	$I_1^1$	-1.5	-1.5	-1.5	-0.5	-0.5	0.5
	$I_2^1$	-0.5	0.5	1.5	0.5	1.5	1.5
$\alpha_1 = 0, \alpha_2 = 1$	$I_1^2$	-1	0	1	-	-	-

the second one is  $\alpha_1 = 0, \alpha_2 = 1$ , in which the number satisfy  $-1 \leq I_1^2 \leq 1$ . They can be characterized by

$$- - \circ - - \bullet - - \bullet - - \circ - -$$

and

$$- - - \circ - - \ddagger - - \circ - - -$$

respectively, where  $\ddagger$  denotes the occupation for a quantum number of 2-string. In Table I, we list all quantum number configurations for  $M = 2$ . The BA equations for these two cases are

$$\begin{aligned} 6 \tan^{-1} x_1^1 &= \pi I_1^1 + \tan^{-1} \frac{x_1^1 - x_2^1}{2}, \\ 6 \tan^{-1} x_2^1 &= \pi I_2^1 + \tan^{-1} \frac{x_2^1 - x_1^1}{2}, \end{aligned} \quad (14)$$

and

$$6 \tan^{-1}(x_1^2/2) = \pi I_1^2, \quad (15)$$

respectively.

**M=3:** In this case the string configuration is characterized by  $\{\alpha_1, \alpha_2, \alpha_3\}$ . In the same way as we did above, we construct a number “ $\alpha_3 : \alpha_2 : \alpha_1$ ”, the maximum value for each digit from left to right is 1, 1, 3 respectively. Then we have 3 string configurations with the condition  $\alpha_1 + 2\alpha_2 + 3\alpha_3 = 3$ , which correspond to the following sequences

$$a : - - - - \bullet - - - \bullet - - - \bullet - - - -$$

$$b : - - - - \circ - - - \bullet - - \circ - - - - \\ - - - - - - - \ddagger - - - - - - -$$

$$c : - - - - - - - \S - - - - - - -$$

where  $a, b, c$  have 1, 3, 1 states respectively,  $\S$  denotes the site for 3-string. And in Table II, we list all quantum number configurations for  $M = 3$ , whose BA equations are

$$\begin{aligned} 6 \tan^{-1} x_1^1 &= \pi I_1^1 + \tan^{-1}(x_1^1 - x_2^1) \\ &\quad + \tan^{-1}(x_1^1 - x_3^1), \\ 6 \tan^{-1} x_2^1 &= \pi I_2^1 + \tan^{-1}(x_2^1 - x_1^1) \\ &\quad + \tan^{-1}(x_2^1 - x_3^1), \\ 6 \tan^{-1} x_3^1 &= \pi I_3^1 + \tan^{-1}(x_3^1 - x_1^1) \\ &\quad + \tan^{-1}(x_3^1 - x_2^1). \end{aligned} \quad (16)$$

TABLE II: All quantum number configurations for  $M = 3$ 

$\alpha_1 = 3, \alpha_2 = 0, \alpha_3 = 0$	$I_1^1$	-1.0	-	-
	$I_2^1$	0	-	-
	$I_3^1$	1.0	-	-
$\alpha_1 = 0, \alpha_2 = 0, \alpha_3 = 1$	$I_1^1$	-1.0	0	1.0
	$I_2^1$	0	0	0
$\alpha_1 = 1, \alpha_2 = 1, \alpha_3 = 0$	$I_1^3$	0	-	-

$$\begin{aligned}
6 \tan^{-1} x_1^1 &= \pi I_1^1 + \tan^{-1}(x_1^1 - x_1^2) \\
&\quad + \tan^{-1}((x_1^1 - x_1^2)/3), \\
6 \tan^{-1} x_1^2 &= \pi I_1^2 + \tan^{-1}(x_1^2 - x_1^1) \\
&\quad + \tan^{-1}((x_1^2 - x_1^1)/3),
\end{aligned} \tag{17}$$

and

$$6 \tan^{-1} x_1^3 = \pi I_1^3. \tag{18}$$

respectively.

As a result we have totally  $C_3^6 = 20$  distinct configurations of quantum number whose Hilbert space is complete.

Then, we compute the eigenvalue for a given quantum number configuration  $\{I_\gamma^n\}$  by solving the BA equations numerically. For the Heisenberg chain, the BA equations can be solved by iteration, for other models, such as the Hubbard model, the BA equations can be solved by a gradient method.

#### IV. MONTE CARLO BETHE ANSATZ

For a system of  $N$  sites, there are  $C_{N/2}^N$  quantum number configurations. This number increases exponentially with the size of the system, so it is impossible to calculate all eigenvalues for a large system, such as  $N > 40$ , under present computer capacity. This restriction can be overcome by a Monte Carlo method. There are many Monte Carlo methods available, and we introduce below a new method that we call Monte Carlo Bethe ansatz. This method is a classical Monte Carlo strategy applied to a quantum problem. The basic idea behind the MCBA method is to simulate the random thermal fluctuation of the system from state to state in quantum number space of the BA solution. This method is not limited by the sign problem, that may show up in the usual quantum Monte Carlo methods.

Since the energy eigenvalues are a function of both  $M$  and of the quantum numbers  $I_\gamma^n$  we can follow a classical Monte Carlo strategy, by sampling the configuration space of  $M$  and  $\{I_\gamma^n\}$ . We now explain how to implement

the Monte Carlo calculation, which follows three steps. Let us assume the present state is  $\mu$  with a corresponding  $M_\mu$  – the number of down spins in state  $\mu$ . From the state  $\mu$  any other state  $\nu$  with  $M_\nu$ , in number of  $C_{N/2}^N - 1$ , can be obtained.

**step one:** first we choose  $M_\nu$ , knowing that the number of states with  $M_\nu$  spins down is  $C_{M_\nu}^N - C_{M_\nu-1}^N$ , thus the probability of selecting  $M_\nu$  is  $(C_{M_\nu}^N - C_{M_\nu-1}^N)/C_{N/2}^N$ .

**step two:** selected  $M_\nu$ , all possible string configurations given  $M_\nu$  are determined from of Eq. (4) which satisfy [3]

$$\sum_{\alpha_1 + \dots + M\alpha_M = M} D(\{\alpha_n\}) = (C_M^N - C_{M-1}^N), \tag{19}$$

with  $D(\{\alpha_n\})$  is the number of states, characterized by the set of quantum numbers  $\{I_\alpha^n\}$  associated with the string configuration  $\{\alpha_n\}$ , and reads

$$D(\{\alpha_n\}) = \prod_{i=1}^M C_{\alpha_j}^{N - \sum_{j=1}^M t_{ij} \alpha_j}. \tag{20}$$

So, in step two, we select a string configuration with the probability  $D(\{\alpha_n\})/(C_M^N - C_{M-1}^N)$ .

**step three:** having determined the string configuration, we then select at random a quantum number configuration, which is the state  $\nu$  we want, for the given string configuration. From the partition function  $Z$ , the probability density for a state  $\mu$  is

$$p_\mu = (N - 2M_\mu + 1)e^{-\beta E_\mu}, \tag{21}$$

where the degeneracy of state  $\mu$  was taken into account. The detailed balance condition tells us the transition probability should satisfy

$$\frac{p_\nu}{p_\mu} = \frac{(N - 2M_\nu + 1)}{(N - 2M_\mu + 1)} e^{-\beta(E_\nu - E_\mu)}. \tag{22}$$

Hence it is possible to use the Metropolis algorithm for the acceptance ratio to accept or reject the state  $\mu$  according to

$$A(\mu \rightarrow \nu) = \begin{cases} \frac{(N - 2M_\nu + 1)}{(N - 2M_\mu + 1)} e^{-\beta(E_\nu - E_\mu)}, & \frac{p_\nu}{p_\mu} < 1 \\ 1, & \text{otherwise.} \end{cases} \tag{23}$$

The MCBA algorithm is complete and the three basic steps are repeated a number of times. After an initial equilibration time, the expectation values can be then estimated as an arithmetic mean over the repeated Markov chain

$$\langle Q \rangle = \frac{1}{N} \sum_{\{\mu\}} Q(\mu). \tag{24}$$

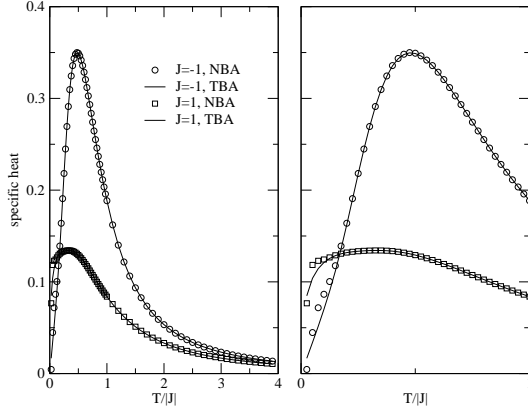


FIG. 1: The specific heat of 24 sites anti-ferromagnetic and ferromagnetic XXX model (points) and the same quantities obtained by TBA (lines).

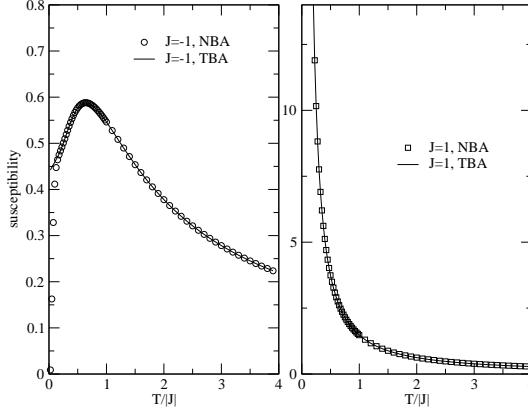


FIG. 2: The susceptibility of 24 sites anti-ferromagnetic (left) and ferromagnetic (right) XXX model (points) and the same quantities obtained by TBA (lines).

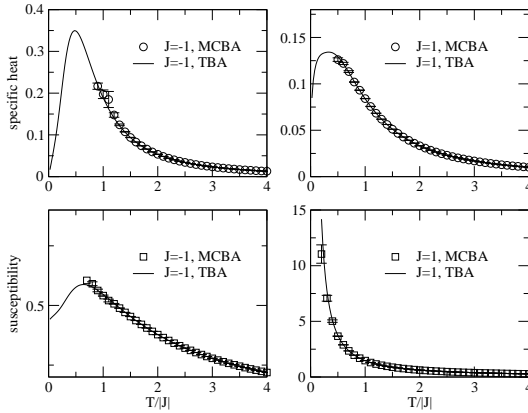


FIG. 3: The specific heat and susceptibility for a 60 sites chain, computed with the MCBA method, is compared with the TBA results (lines) both for the anti-ferromagnetic (circles) and ferromagnetic (squares) cases.

TABLE III: Specific heat and susceptibility of ferromagnetic XXX model obtained by thermodynamic Bethe ansatz (TBA), numerical Bethe ansatz (NBA) solution of 24 sites, and Bethe ansatz based Monte Carlo (MCBA) approach for 60 sites system.

	$T/J$	TBA	NBA	MCBA
$C_v$	0.5	0.129178	0.129197	$0.1261 \pm 0.0019$
	0.6	0.121671	0.121688	$0.1220 \pm 0.0012$
	0.7	0.112363	0.112379	$0.1132 \pm 0.0009$
	0.8	0.102496	0.102511	$0.1019 \pm 0.0003$
	0.9	0.092861	0.092875	$0.0931 \pm 0.0002$
	1.0	0.083875	0.083887	$0.0840 \pm 0.00017$
	1.5	0.051111	0.051117	$0.05112 \pm 0.00004$
	2.0	0.03256	0.03260	$0.03326 \pm 0.00002$
	2.5	0.023088	0.023090	$0.02308 \pm 0.00001$
	3.0	0.016876	0.016878	$0.01687$
$\chi$	0.5	3.7378	3.742446	$3.669 \pm 0.027$
	0.6	2.90686	2.909917	$2.8914 \pm 0.0139$
	0.7	2.35856	2.360709	$2.3458 \pm 0.0039$
	0.8	1.97323	1.974817	$1.9613 \pm 0.0044$
	0.9	1.68953	1.690744	$1.6902 \pm 0.0028$
	1.0	1.473032	1.473986	$1.47509 \pm 0.00180$
	1.5	0.882613	0.882996	$0.88316 \pm 0.00016$
	2.0	0.622855	0.623056	$0.62299 \pm 0.00010$
	2.5	0.479082	0.479205	$0.47908 \pm 0.00007$
	3.0	0.388433	0.388516	$0.38848 \pm 0.00004$

## V. SPECIFIC HEAT AND SUSCEPTIBILITY

In order to check the validity of our approaches, we apply these two methods to the study of the specific heat and of the magnetic susceptibility of the anti-ferromagnetic and ferromagnetic Heisenberg models.

For the present model, however, because of the degeneracy in each set of quantum number configuration, Eq. (8) should be revised according to the property of the operator. For example, the internal energy and magnetization are

$$\begin{aligned} \langle E \rangle &= \frac{1}{Z} \sum_{\mu} (N - 2M_{\mu} + 1) E_{\mu} e^{-\beta E_{\mu}}, \\ \langle M \rangle &= \frac{1}{Z} \sum_{\mu} \sum_{M_{\mu}^z = -N/2 + M_{\mu}}^{N/2 - M_{\mu}} 2M_{\mu}^z e^{-\beta E_{\mu}}. \end{aligned} \quad (25)$$

where  $Z = \sum_{\mu} (N - 2M_{\mu} + 1) e^{-\beta E_{\mu}}$ . From thermodynamics it is easy to have the expression for specific heat and magnetic susceptibility per site

$$\begin{aligned} C &= \frac{\beta^2}{N} (\langle E^2 \rangle - \langle E \rangle^2), \\ \chi &= \frac{\beta}{N} (\langle M^2 \rangle - \langle M \rangle^2) \end{aligned} \quad (26)$$

We apply NBA to 24-site system and MCBA to 60-site system, respectively. The later has  $C_{30}^{60}$  different quan-

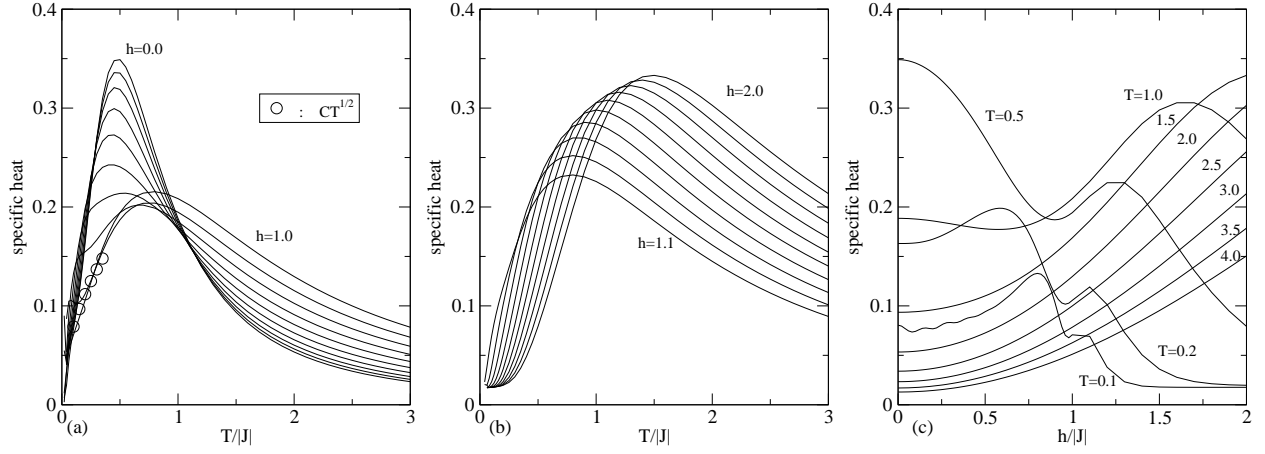


FIG. 4: The specific heat of the anti-ferromagnetic Heisenberg model for different values of the external field: (a)  $h = 0, 0.2, 0.3, \dots, 1.0$ ; (b)  $h = 1.1, 1.2, \dots, 2.0$ ; (c) specific heat as a function of  $h$  for different temperature  $T = 0.1, 0.2, \dots, 4.0$ . In panel (a) of fit to the law  $C \propto T^{1/2}$ , for  $h=1.0$ , is given at low temperatures.

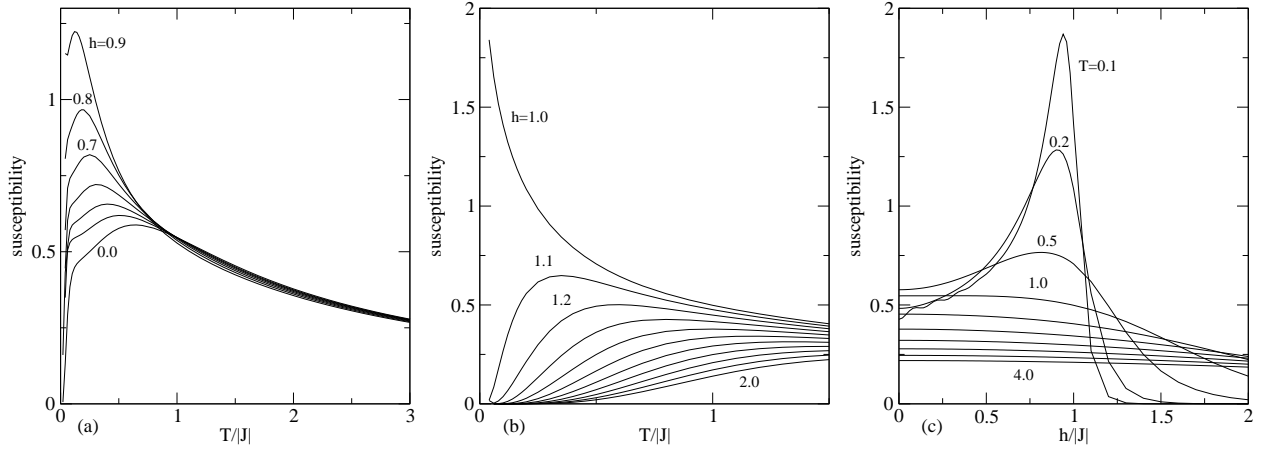


FIG. 5: The magnetic susceptibility of the anti-ferromagnetic Heisenberg model for different values of the external field: (a)  $h = 0, 0.4, 0.5, \dots, 0.9$ ; (b)  $h = 1.0, 1.2, \dots, 2.0$ ; (c) magnetic susceptibility as a function of  $h$  for different temperature  $T = 0.1, 0.2, \dots, 4.0$ .

tum number configurations, hence it is impossible to calculate all the eigenvalues of the system.

In Figs. 1 and 2, we show the specific heat and the magnetic susceptibility, for a 24-site system, obtained from NBA and compare our results with those obtained from TBA. It is clear that the two results match. In Fig 3, we show the specific heat and the magnetic susceptibility, for a 60-site system obtained from MCBA together with the results from TBA. They both agree to each other except at low temperature. In Table V, we compare, for the ferromagnetic case, the two methods we introduced here with TBA, giving the explicit numerical values. It is clear that our methods work very well for the present model. Hence our conclusion is that for small systems, such as  $N \leq 38$ , and for the Heisenberg chain, it is possible to compute all eigenvalues and to obtain all possible

thermodynamic quantities of interest by using Eq. (8). For temperatures larger than the finite size energy gap our results agree with TBA results exactly. For larger systems, however, results can still be obtained by using the MCBA method.

Now we study the thermodynamics of the model in the presence of a magnetic field by NBA, which has also been studied by Klümper [26]. In Fig. 4 and Fig. 5, the results for the specific heat and the magnetic susceptibility of the anti-ferromagnetic case are shown for various magnetic fields. It is clear from these two figures that there are two different behaviors at low temperature, separated by the saturation field  $h_c = 1.0$  at the ground state. In order to understand better this behavior of the antiferromagnetic case, let us use the mapping between the Heisenberg model and the spinless fermion

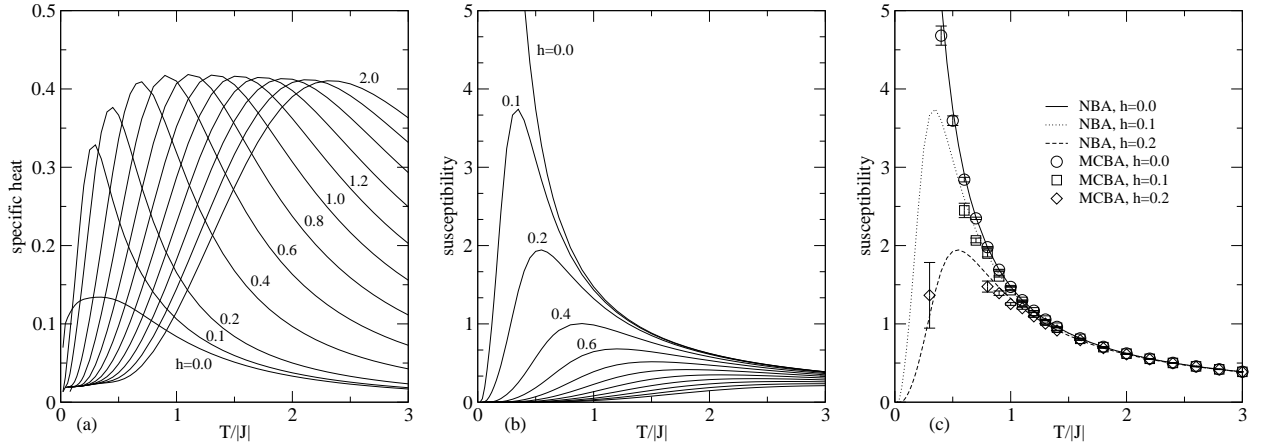


FIG. 6: The specific heat(a) and the magnetic susceptibility(b) ferromagnetic Heisenberg model as a function of temperature for different values of external field  $h = 0.0, 0.1, 0.2, \dots, 2.0$ , obtained by NBA. (c). The susceptibility of ferromagnetic Heisenberg model for  $h = 0.0, 0.1, 0.2$ , obtain by NBA and MCBA respectively.

model. This mapping is achieved by the Jordan-Wigner transformation [29], and Hamiltonian (1) can be written as

$$\mathcal{H} = -\frac{J}{2} \sum_{l=1}^N (f_l^\dagger f_{l+1} + f_{l+1}^\dagger f_l) + J \sum_{l=1}^N (n_l - \frac{1}{2})(n_{l+1} - \frac{1}{2}). \quad (27)$$

where the spinless fermion operators  $f_l^\dagger, f_l$  obey the usual anti-commutation relation,  $n_l$  is the usual local number operator. When  $h < h_c$ , the system is not fully polarized, that is  $\sum_{l=1}^N n_l > 0$ , hence we always have two Fermi points  $\pm k_F$  at the ground state. The dispersion relation of low-lying excitations is dominated by the linear- $k$  dependence, hence we still have the Fermi-liquid like specific heat:  $C \propto T$  at low temperatures. If  $h \geq h_c$ , however, and from the point view of spinless fermions, we have  $\sum_{l=1}^N n_l = 0$ , and the dispersion relation becomes  $k^2$ , because of the  $\cos k$  dispersion-relation for the fermions in the lattice. Hence, the specific heat manifest a  $T^{1/2}$  behavior at sufficiently low temperature for  $h = h_c$ , which can be seen in Fig. 4 (open circles). Moreover, the magnetic susceptibility presents a strong peak for  $h = h_c$ , when  $T \rightarrow 0$  [see Fig. 5, panel (c)]. This strong magnetic response is associated with a change in the nature of the elementary excitations when the line  $h = h_c$  is crossed at zero temperature. Indeed, at  $T = 0$  and  $h_c = 1.0$ , the system manifest infinite susceptibility, as can be seen from Fig. 5, panel (b). We attribute it due to the degeneracy between the state of  $[N-1, 1]$  and  $[N]$ , and a small magnetic field can fully polarize the system. The phase with  $h \geq h_c$  share anti-ferromagnetic-like behavior [Fig. 6, panel (b)], while for  $h < h_c$ , the susceptibility shows a logarithm singularity [26].

For the ferromagnetic case the specific heat and the magnetic susceptibility are plotted in Fig. 6, for different

values of the magnetic field. As is known, if  $h = 0$  the ground state of the ferromagnetic case is highly degenerate with  $S = N/2, S_z = -S, -S+1, \dots, S$  and a very small  $h$  can fully polarized the system. So it is easy to understand why zero temperature susceptibility is infinite. After it is magnetized (in the presence of small  $h$ ), however, the susceptibility should be zero. This behavior is seen in Fig. 6, panel (b). We also show, in Fig. 6, panel (c), the susceptibility obtained by MCBA. Both the results of the two methods agree with each other perfectly.

## VI. SUMMARY

In summary, we presented two numerical approaches to discuss the thermodynamics of Bethe ansatz solvable models. The first one is the numerical Bethe ansatz which works very well for a small system. We think it is possible to obtain all eigenvalues of a system up to size  $L = 38$ , for the Heisenberg model. For a relatively larger system, we also find that the Monte Carlo simulation in quasi-momentum space works well in the moderate and high temperature regions. At low temperatures the present selection method is not excellent, and a better one is required. The discovery of such a method is a challenging and interesting research problem.

There are many physical quantities of interest at finite temperature which are still not well understood, such as spin stiffness of XXZ model, important to understand the transport properties, because of the complex form of the thermodynamic equations. Our methods provide a new route to compute all these quantities directly from the Bethe ansatz equations.

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